

FINAL REPORT

Submitted to

National Aeronautics and Space Administration

Research Performed under Cooperative Agreement NCC1-80

July 1983 - April 2000

By

Investigators: PI: Dr. D. Chris Benner

Department of Physics

The College of William and Mary

Williamsburg, Virginia 23187-8795

Telephone: (757) 221-3531/(757)-864-5699

E mail: dcbenn@facstaff.wm.edu

Co-I: Dr. Malathy Devi Venkataraman

Department of Physics

The College of William and Mary

Williamsburg, Virginia 23187-8795

Telephone: (757) 221-3531/(757)-864-5521

E mail: m.d.venkataraman@larc.nasa.gov

Title: High Resolution Spectroscopy to Support Atmospheric Measurements

The major research activities performed during the cooperative agreement enhanced our spectroscopic knowledge of molecules of atmospheric interest such as carbon dioxide, water vapor, ozone, methane, and carbon monoxide, to name a few. Measurements were made using the NASA Langley Tunable Diode Laser Spectrometer System (TDL) and several Fourier Transform Spectrometer Systems (FTS) around the globe. The results from these studies made remarkable improvements in the line positions and intensities for several molecules, particularly ozone and carbon dioxide in the 2 to 17- μ m spectral region. Measurements of pressure broadening and pressure induced line shift coefficients and the temperature dependence of pressure broadening and pressure induced line shift coefficients for infrared transitions of ozone, methane, and water vapor were also performed. Results from these studies have been used for retrievals of stratospheric gas concentration profiles from data collected by several Upper Atmospheric Research satellite (UARS) infrared instruments as well as in the analysis of high resolution atmospheric spectra such as those acquired by space-based, ground-based, and various balloon- and aircraft-borne experiments. Our results made significant contributions in several updates of the HITRAN (High resolution TRANsmission) spectral line parameters database. This database enjoys worldwide recognition in research involving diversified scientific fields.

The high lights of the results from this cooperative agreement include:

1. **Atlas of Ozone Spectral Parameters from Microwave to Medium Infrared:** J.-M. Flaud, C. Camy-Peyret, C. P. Rinsland, M. A. H. Smith and V. Malathy Devi, Academic Press, Inc. San Diego, CA 1990.
2. **Intensities and Collision-Broadening Parameters from Infrared Spectra: An Update.** M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, L. S. Rothman and K. Narahari Rao, in **Spectroscopy of the Earth's Atmosphere and Interstellar Medium**, Ed. K. Narahari Rao and Alfons Weber, Academic Press, Inc. San Diego, CA 1992..

3. Infrared Spectroscopy of the CO₂ Molecule. V. Malathy Devi, D. Chris Benner, C. P. Rinsland, M. A. H. Smith, and D. S. Parmar. in Recent Research Development in Geophysical Research, 1 (1996). Ed. S. G. Pandali, pp. 119-148, Research Signpost, Trivandrum, India (1996).
4. 75 Research papers have been published in several reputable journals (see list attached).
5. More than 85 oral / poster presentations have been given in several International Spectroscopic Symposia /Conferences held in the US and abroad.

Brief descriptions of the various projects:

1. Because of its very important contribution to atmospheric absorption in the infrared, the vibration-rotation spectrum of CO₂ has been the subject of numerous high-resolution studies. We undertook a comprehensive and extensive analysis of accurate positions and intensities of individual absorption lines of CO₂ in the 1800 to 4000 cm⁻¹ spectral region. The analyses of several high resolution long path absorption spectra of a natural sample of CO₂ have yielded accurate positions and intensities of over 10000 transitions belonging to more than 200 vibration rotation bands of eight isotopic species of CO₂. Pressure-broadening and pressure-induced line shift coefficients in the v₃ fundamental band in the 4.3 μm region, and in the laser band regions around 9-11 μm, as well as line mixing coefficients in several Q branches in the 2 to 5 μm spectral region were determined. These results were obtained by analyzing high-resolution Fourier transform laboratory absorption spectra.
2. Methane is another molecule of importance to atmospheric studies. Due to the high methane abundance (~1.6 ppmv) in the atmosphere, even lines belonging to isotopic methane (such as ¹³CH₄ and ¹²CH₃D) contribute significant absorption in many regions of atmospheric spectra. Accurate measurements of spectroscopic parameters such as pressure-broadening coefficients, pressure-induced line-shift coefficients, line mixing coefficients and their temperature dependence are needed for accurate simulations of methane features in atmospheric spectra.

Based upon these requirements, we have recorded more than 300 high-resolution laboratory FTS spectra of CH₄ and its isotopes. The majority of these spectra have been obtained at 0.005 to 0.01 cm⁻¹ resolution using the McMath-Pierce FTS. About 100 of these spectra (CH₄) were recorded

with the FTS at LPM (Laboratoire de Photophysique Moleculaire, CNRS, Orsay), France. We have determined air- and N₂-broadening and shift coefficients at room temperature for a large number of lines in the 7.5- μ m, 3.3- μ m, and 2.3- μ m bands of methane. Temperature dependence of these coefficients has been determined in the 7.5- μ m region and in the 2.3- μ m region. O₂-broadening and shift coefficients for CH₄ have been experimentally determined in the 3.3- μ m region at room temperature.

Pressure broadening coefficients of ¹²CH₄, ¹³CH₄ and ¹²CH₃D molecules in several spectral regions including the fundamental, combination and overtone bands have been determined using TDL and FTS instruments. First measurements of the temperature dependence exponents of broadening and shift coefficients for hundreds of spectral lines in the v₄ fundamental bands of ¹²CH₄ and ¹³CH₄ were measured from analyzing spectra obtained with a FTS in conjunction with a coolable absorption cell.

We determined the temperature dependence of air-broadening, pressure shifting and line mixing for ¹²CH₄ transitions in the v₃ band region by analyzing high-resolution spectra of methane recorded with 3 Fourier transform spectrometers. More than 60 laboratory absorption spectra of ¹²CH₄, ¹³CH₄ and ¹²CH₃D obtained at various temperatures (-60⁰C to +25⁰C) were used in the analysis. The spectra were recorded with the McMath FTS (0.01 cm⁻¹ resolution), with the FTS at LPM (Laboratoire de Photophysique Moleculaire, CNRS, Orsay-France) with 0.003 cm⁻¹ resolution and with the FTS at the Pacific Northwest National Laboratory (PNNL) with 0.0015 cm⁻¹. Absorption cells with path lengths from 1.7 cm to 2500 cm and pressures from less than one torr to more than 500 torr were used in obtaining the spectra. The line mixing model incorporated into the least-squares fitting procedure determines separate relaxation matrix coefficients related to air-broadening and self-broadening. Using these techniques, it is possible to determine the temperature dependence exponents for the broadening, shifting and the off-diagonal relaxation matrix coefficients associated with line mixing. Our results so far include the P(11) to P(3) manifolds of methane. These results will facilitate developing a more accurate database of methane positions, intensities, broadening, shifting, line mixing and the temperature dependence of broadening, shifting and line mixing coefficients for the v₃ region.

Accurate laboratory measurements of positions, intensities, pressure broadening and pressure induced shift coefficients of CH₃D lines are crucial for quantitative analysis (e.g., determination of CH₃D abundance and D/H ratio) of the spectral signatures of this molecule observed in the terrestrial and planetary atmospheres. The multispectrum fitting technique capable of interpreting the line mixing effects have successfully been applied in the analyses of the triad region (ν_3 , ν_5 and ν_6 bands) of ¹²CH₃D in the 6-10 μ m spectral region.

We recently presented detailed measurements of ten methane spectra recorded at 0.011 cm⁻¹ resolution in the following MOPITT (Measurements Of Pollution In The Troposphere) spectral regions: 4265-4305 cm⁻¹ (the MOPITT CO channel) and 4350-4500 cm⁻¹ (the MOPITT CH₄ channel). These two spectral channels are part of the crowded methane “octad region” containing eight overtone and combination bands. These spectra were recorded using the MaMath-Pierce FTS. Using the multispectrum fitting technique we have measured accurate line intensities, self- and air-broadened half width and pressure shift coefficients for more than 1000 methane transitions.

3. Water vapor plays a crucial role in atmospheric chemistry. Many remote sensing experiments utilize the pure rotation and vibration-rotation bands of water vapor for soundings of H₂O in the Earth's atmosphere. We measured transitions belonging to several infrared bands of H₂¹⁶O and its deuterated species (H₂¹⁸O, HDO and D₂O) using both the TDL and FTS systems. Using our heatable mutipass absorption cell, we have recorded ‘hot’ water spectra to determine the variation of the width and shift coefficients of water vapor lines (broadened with foreign gases such as air, N₂) in the ν_1 and ν_3 fundamentals near the 3- μ m spectral region.

4. Determination of accurate line positions, assignments, and intensities of the normal (¹⁶O₃) and ¹⁸O- and ¹⁷O- isotopomers of ozone in the 2 to 17 μ m spectral regions has been the major focus of our research during the past decade. We have recorded numerous high-resolution (0.0027 to 0.01 cm⁻¹) room temperature laboratory absorption spectra of nearly pure ozone since 1984. We used the McMath-Pierce FTS as well as the Tunable Diode Laser spectrometer at NASA Langley Research Center to obtain hundreds of ozone spectra. Analyses of the spectra were performed collaborating

with investigators from Laboratoire de Photophysique Moleculaire in Orsay, France. Several of the earlier ozone spectra recorded during 1984 to 1988 resulted in improved line positions and intensities for the fundamental bands of $^{16}\text{O}_3$, ^{18}O - monosubstituted species $^{16}\text{O}^{18}\text{O}^{16}\text{O}$, $^{16}\text{O}^{16}\text{O}^{18}\text{O}$, ^{17}O - monosubstituted species $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ and $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ as well as the overtone, combination, and a number of 'hot' bands of $^{16}\text{O}_3$. The results from these studies were used to update the line parameters in the 1992 HITRAN database. The new line parameters significantly improved the retrievals of stratospheric ozone and other trace gases from infrared remote sensing measurements.

Laboratory measurements of nitrogen and oxygen broadening and shift coefficients of ozone are particularly important to verify theoretical calculations which are useful to predict values for lines not measured by experiments. In 1990 and 1991 we recorded a large number of high resolution spectra of pure ozone and lean mixtures of ozone broadened with dry air at various temperatures from room temperature down to -63°C . These spectra were recorded using the McMath-Pierce FTS at Kitt Peak and the 50cm long coolable absorption cell. In addition to covering the ozone fundamental bands, ν_1 and ν_2 , these spectra also cover the combination band $\nu_1 + \nu_3$. We have made the first air broadening and shift measurements for over 440 lines in the ν_1 band and over 350 lines in the ν_2 band. The pressure induced shift coefficients and the temperature dependence of the shift coefficients for these ozone bands has never been determined before.

In September 1999 we recorded 8 high-resolution spectra of normal ($^{16}\text{O}_3$) and isotopic ($^{16}\text{O}^{18}\text{O}^{16}\text{O}$, $^{16}\text{O}^{16}\text{O}^{18}\text{O}$, $^{18}\text{O}^{16}\text{O}^{18}\text{O}$, $^{18}\text{O}^{18}\text{O}^{16}\text{O}$, $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ and $^{18}\text{O}_3$) species of ozone. These spectra were recorded at a resolution of 0.002 cm^{-1} using the Denver University Bruker IFS 120 HR Fourier transform spectrometer. The wavenumber range of these spectra is 1988 to 2550 cm^{-1} . This spectral region involves the 2 overtone bands $2\nu_1$ and $2\nu_3$ as well as the combination band $\nu_1 + \nu_3$.

Note: We would like to point out that not all the work undertaken in this cooperative agreement is included above. More details may be available through the publications listed below.

Research Publications resulting from this Cooperative Agreement :

1. Simultaneous Stratospheric Measurements of H₂O, HDO, and CH₄ from Balloon-Borne and Aircraft Infrared Solar Absorption Spectra and Tunable Diode Laser Laboratory Spectra of HDO.
C. P. Rinsland, A. Goldman, V. Malathy Devi, B. Fridovich, D. G. S. Snyder, G. D. Jones, F. J. Murcray, D. G. Murcray, M. A. H. Smith, R. K. Seals, Jr., M. T. Coffey, and W. G. Mankin
J. Geophy. Res. 89, 7259 (1984).
2. Atlas of High Resolution Infrared Spectra of Carbon Dioxide: February 1984 Edition.
C. P. Rinsland, D. Chris Benner, V. Malathy Devi, P. S. Ferry, C. H. Sutton, and D. J. Richardson
NASA Tech. Memo. 85764 (1984).
3. Atlas of High Resolution Infrared Spectra of Carbon Dioxide.
C. P. Rinsland, D. Chris Benner, V. Malathy Devi, P. S. Ferry, C. H. Sutton, and D. J. Richardson
Applied Optics 23, 2051 (1984).
4. Absolute intensity measurements of CO₂ bands in the 2395-2680 cm⁻¹ region.
V. Malathy Devi, C. P. Rinsland, and D. Chris Benner
Applied Optics 23, 4067 (1984).
5. Measurements of absolute line intensities in carbon dioxide bands near 5.2 μ m.
C. P. Rinsland, D. Chris Benner, and V. Malathy Devi
Applied Optics 24, 1644 (1985).
6. Infrared Measurements of Atmospheric Ethane (C₂H₆) from Aircraft and Ground-based Solar Absorption Spectra in the 3000 cm⁻¹ Region.
M. T. Coffey, W. G. Mankin, A. Goldman, C. P. Rinsland, G. A. Harvey, V. Malathy Devi, and G. M. Stokes
Geophy. Res. Lett. 12, 199 (1985).
7. Tentative identification of the 780-cm⁻¹ v₄ Band Q branch of Chlorine Nitrate in High Resolution Solar Absorption Spectra of the stratosphere.

C. P. Rinsland, A. Goldman, D. G. Murcray, F. J. Murcray, F. S. Bonomo, R. D. Blatherwick, V. Malathy Devi, M. A. H. Smith, and P. L. Rinsland
J. Geophys. Res. 90, 7931 (1985).

8. Identification of ^{18}O -isotopic Lines of Ozone in Infrared Ground-based Solar Absorption Spectra.
 C. P. Rinsland, V. Malathy Devi, J. -M. Flaud, C. Camy-Peyret, M. A. H. Smith, and G. M. Stokes
J. Geophys. Res. 90, 10719 (1985).

9. Measurements of $^{12}\text{CH}_4$ ν_4 band halfwidths using a tunable diode laser system and a Fourier transform spectrometer.
 V. Malathy Devi, C. P. Rinsland, M. A. H. Smith, and D. Chris Benner
Applied Optics 24, 3321 (1985).

10. Tunable diode laser measurements of widths of air- and nitrogen-broadened lines in the ν_4 band of $^{13}\text{CH}_4$.
 V. Malathy Devi, C. P. Rinsland, M. A. H. Smith, and D. Chris Benner
Applied Optics 24, 3321 (1985).

11. Tunable diode laser measurements of N_2 - and air-broadened halfwidths: Lines in the $(\nu_4 + \nu_5)^0$ band of $^{12}\text{C}_2\text{H}_2$ near $7.4 \mu\text{m}$
 V. Malathy Devi, D. Chris Benner, C. P. Rinsland, M. A. H. Smith, and B. D. Sidney
J. Mol. Spectrosc. 114, 49 (1985).

12. Tunable diode laser measurements of widths of air- and N_2 - broadened lines in the ν_2 band of D_2O .
 V. Malathy Devi, C. P. Rinsland, D. Chris Benner, and M. A. H. Smith
Applied Optics 25, 336 (1986).

13. Absolute Line Intensities in CO_2 Bands Near $4.8 \mu\text{m}$.
 C. P. Rinsland, D. Chris Benner, and V. Malathy Devi
Appl. Opt. 25, 1204 (1986).

14. Absolute intensities and self-, N_2 -, and air-broadened Lorentz halfwidths for selected lines in the ν_3 band of $^{12}\text{CH}_3\text{D}$ from measurements with a tunable diode laser spectrometer.

V. Malathy Devi, C. P. Rinsland, D. Chris Benner, M. A. H. Smith, and K. B. Thakur
Applied Optics 25, 1848 (1986).

15. Tunable diode laser measurements of air-broadened linewidths in the ν_6 band of H_2O_2 .
 V. Malathy Devi, C. P. Rinsland, M. A. H. Smith, D. Chris Benner, and Bernard Fridovich
Applied Optics 25, 1844 (1986).

16. Diode Laser Measurements of Air and Nitrogen Broadening in the ν_2 bands of HDO, H_2^{16}O , and H_2^{18}O .
 V. Malathy Devi, D. Chris Benner, C. P. Rinsland, M. A. H. Smith, and B. D. Sidney
J. Mol. Spectrosc. 117, 403 (1986).

17. Absolute line intensity measurements in the ν_2 bands of HDO, D_2O using a tunable diode laser spectrometer.
 K. B. Thakur, C. P. Rinsland, M. A. H. Smith, D. Chris Benner, and V. Malathy Devi
J. Mol. Spectrosc. 120, 239 (1987).

18. The ν_1 and ν_3 Bands $^{16}\text{O}^{16}\text{O}^{18}\text{O}$: Line Positions and Intensities.
 J. -M. Flaud, C. Camy-Peyret, V. Malathy Devi, C. P. Rinsland, and M. A. H. Smith
J. Mol. Spectrosc. 118, 334 (1986).

19. The Hybrid-Type Bands ν_1 and ν_3 of $^{16}\text{O}^{16}\text{O}^{18}\text{O}$: Line Positions and Intensities.
 C. Camy-Peyret, J. -M. Flaud, A. Perrin, V. Malathy Devi, C. P. Rinsland, and M. A. H. Smith
J. Mol. Spectrosc. 118, 345 (1986).

20. Q branches of the ν_7 Fundamental of Ethane (C_2H_6): Integrated Intensity Measurements for Atmospheric Measurement Applications.
 C. P. Rinsland, Gale A. Harvey, V. Malathy Devi, K. B. Thakur, Joel S. Levine, and M. A. H. Smith
Appl. Opt. 25, 2872 (1986).

21. Analysis of High Resolution Fourier Transform Spectra of the ν_6 Band of Carbonyl Fluoride.
 K. B. Thakur, K. Narahari Rao, R. R. Friedl, C. P. Rinsland, and V. Malathy Devi
J. Mol. Spectrosc. 122, 182 (1987).

22. Diode Laser Measurements of Intensities and Halfwidths in the ν_6 band of $^{12}\text{CH}_3\text{D}$.
 V. Malathy Devi, D. Chris Benner, C. P. Rinsland, M. A. H. Smith, and K. B. Thakur
J. Mol. Spectrosc. 122, 182 (1987).

23. The ν_1 and ν_3 Bands of $^{18}\text{O}_3$ and $^{18}\text{O}^{16}\text{O}^{18}\text{O}$: Line Positions and Intensities.
 J. -M. Flaud, C. Camy-Peyret, V. Malathy Devi, C. P. Rinsland, and M. A. H. Smith
J. Mol. Spectrosc. 122, 221 (1987).

24. The ν_1 and ν_3 Bands of $^{16}\text{O}_3$: Line Positions and Intensities.
 J. -M. Flaud, C. Camy-Peyret, V. Malathy Devi, C. P. Rinsland, and M. A. H. Smith
J. Mol. Spectrosc. 124, 209 (1987).

25. Line Position and Intensities for $\nu_1 + \nu_2$ and $\nu_2 + \nu_3$ Bands of $^{16}\text{O}_3$.
 V. Malathy Devi, J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, and M. A. H. Smith
J. Mol. Spectrosc. 125, 174 (1987).

26. Air-Broadened and Nitrogen-Broadened Lorentz Width Coefficients and Pressure Shift Coefficients in the ν_4 and ν_2 bands of $^{12}\text{CH}_4$.
 C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and D. Chris Benner
Applied Optics 27, 631 (1988).

27. Air-Broadened Lorentz Halfwidths and Pressure-Induced Line Shifts in the ν_4 band of $^{13}\text{CH}_4$.
 V. Malathy Devi, C. P. Rinsland, M. A. H. Smith, and D. Chris Benner
Applied Optics 27, 2296 (1988).

28. Measurements of Air-Boadened and Nitrogen-Broadened Halfwidths and Shifts of Ozone Lines Near 9 μm .
 M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, D. Chris Benner, and K. B. Thakur
J. Opt. Soc. Am. B 5, 585 (1988).

29. Absolute intensities of CO_2 Lines in the 3140 to 3410 cm^{-1} Spectral Region.
 D. Chris Benner, V. Malathy Devi, and C. P. Rinsland
Applied Optics 27, 1588 (1988).

30. Vibrational and Rotational Spectra of Normal Ozone for the (0,1,0) and (0,2,0) States.

H. M. Pickett, E. A. Cohen, L. R. Brown, C. P. Rinsland, M. A. H. Smith, V. Malathy Devi, A. Goldman, A. Barbe, B. Carli, and M. Carlotti
J. Mol. Spectrosc. 128, 151 (1988).

31. Line Positions and Intensities of the $2\nu_3$, $\nu_1 + \nu_3$ and $2\nu_1$ Bands of $^{16}\text{O}_3$.
 C. P. Rinsland, M. A. H. Smith, J. -M. Flaud, C. Camy-Peyret, and V. Malathy Devi
J. Mol. Spectrosc. 130, 204 (1988).

32. The ν_2 bands of $^{16}\text{O}^{18}\text{O}^{16}\text{O}$ and $^{16}\text{O}^{16}\text{O}^{18}\text{O}$: Line Positions and Intensities.
 J. -M. Flaud, C. Camy-Peyret, A. N'Gom, V. Malathy Devi, C. P. Rinsland, and M. A. H. Smith
J. Mol. Spectrosc. 133, 217 (1989).

33. Line parameters for $^{16}\text{O}_3$ bands in the 7- μm region.
 J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, M. A. H. Smith, and V. Malathy Devi
J. Mol. Spectrosc. 134, 106 (1989).

34. Measurements of Argon-Broadened Lorentz width and pressure-induced line shift coefficients in the ν_4 band of $^{12}\text{CH}_4$.
 C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and D. Chris Benner
Applied Optics 28, 211 (1989).

35. The 3.6 μm Region of Ozone: Line Positions and Intensities.
 M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, J. -M. Flaud, and C. Camy-Peyret
J. Mol. Spectrosc. 139, 171 (1990).

36. Line Parameters for Ozone Bands in the 4.8- μm Spectral Region.
 J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, M. A. H. Smith, V. Malathy Devi, and A. Goldman
J. Mol. Spectrosc. 139, 343 (1990).

37. The 3.3 μm Bands of Ozone: Line Positions and Intensities.
 C. Camy-Peyret, J. -M. Flaud, M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, J. J. Plateaux, and A. Barbe
J. Mol. Spectrosc. 141, 134 (1990).

38. The ν_2 bands of $^{18}\text{O}_3$, $^{18}\text{O}^{16}\text{O}^{18}\text{O}$ and $^{16}\text{O}^{18}\text{O}^{18}\text{O}$: Line Positions and Intensities.

A. Perrin, A. -M. Vasserot, J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, M. A. H. Smith, and V. Malathy Devi, *J. Mol. Spectrosc.* 143, 311(1990).

39. Line Positions and Intensities for the $\nu_2+3\nu_3$ Band of $^{16}\text{O}_3$ around 7- μm . V. Malathy Devi, A. Perrin, J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, and M. A. H. Smith *J. Mol. Spectrosc.* 143, 381(1990).

40. Improved Line Parameters for Ozone Bands in the 10- μm Spectral Region. J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and A. Goldman *Appl. Opt.* 29, 3667 (1990).

41. Measurements of Air-, N_2 -, and O_2 - broadened Halfwidths and pressure-induced Line Shifts in the ν_3 band of $^{13}\text{CH}_4$. V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsland *Applied Optics* 30, 287 (1991); *Erratum*: *Applied Optics* 30, 2928 (1991).

42. Analysis of High Resolution Spectrum of Acetylene in the 2.4 μm Region. R. D'Cunha, Y. A. Sarma, G. Guelachvili, R. Farrenq, Q. Kou, V. Malathy Devi, D. Chris Benner, and K. Narahari Rao *J. Mol. Spectrosc.* 148, 213 (1991).

43. Measurements of Lorentz air-broadening coefficients and relative intensities in the H_2^{16}O pure rotational and ν_2 bands from long horizontal path atmospheric spectra. C. P. Rinsland, A. Goldman, M. A. H. Smith, and V. Malathy Devi *Appl. Opt.* 30, 1427 (1991).

44. Measurements of self-broadening of infrared absorption lines of ozone. M. A. H. Smith, C. P. Rinsland, and V. Malathy Devi *J. Mol. Spectrosc.* 147, 142 (1991).

45. The ν_2 bands of $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ and $^{16}\text{O}^{16}\text{O}^{17}\text{O}$: Line Positions and Intensities. C. P. Rinsland, M. A. H. Smith, V. Malathy Devi, A. Perrin, J. -M. Flaud, and C. Camy-Peyret *J. Mol. Spectrosc.* 149, 474 (1991).

46. Measurements of Lorentz-broadening Coefficients and Pressure-Induced Line Shift Coefficients in the ν_2 band of $D_2^{16}O$.
C. P. Rinsland, M. A. H. Smith, V. Malathy Devi, and D. Chris Benner
J. Mol. Spectrosc. 150, 173 (1991).

47. Measurements of Lorentz-broadening Coefficients and Pressure-Induced Line Shift Coefficients in the ν_2 band of $HD^{16}O$.
C. P. Rinsland, M. A. H. Smith, V. Malathy Devi, and D. Chris Benner
J. Mol. Spectrosc. 150, 640 (1991).

48. Measurements of Pressure Broadening and Pressure Shifting by Nitrogen in the 4.3- μm band of $^{12}C^{16}O_2$.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsland
J. Quant. Spectrosc. Radiat. Transfer 48, 581 (1992).

49. Temperature Dependence of Broadening and Shift Coefficients of Methane Lines in the ν_4 band.
M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, and D. Chris Benner
Spectrochimica Acta 48A, 1257 (1992).

50. The ν_1 and ν_3 bands of $^{16}O^{17}O^{16}O$: Line Positions and Intensities.
M. Heyart, A. Perrin, J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, M. A. H. Smith, and V. Malathy Devi
J. Mol. Spectrosc. 156, 210 (1992).

51. Measurements of Pressure Broadening and Pressure Shifting by Nitrogen in the ν_1 and ν_3 bands of $H_2^{16}O$.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsland
J. Mol. Spectrosc. 155, 333 (1992).

52. The HITRAN molecular database: Editions of 1991 and 1992.
L. S. Rothman, R. R. Gamache, R. H. Tipping, C. P. Rinsland, M. A. H. Smith, D. Chris Benner, V. Malathy Devi, J. -M. Flaud, C. Camy-Peyret, A. Perrin, A. Goldman, S. T. Massie, L. R. Brown, and R. A. Toth
J. Quant. Specrosc. Radiat. Transfer 48, 469 (1992).

53. Intensities and Collision Broadening Parameters from Infrared Spectra: An update.
M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, L. S. Rothman, and K. Narahari Rao
In: *Spectroscopy of the Earth's Atmosphere and Interstellar Molecules*, Eds. K. Narahari Rao and A. Weber, Cambridge, Mass. Academic Press, Inc. (1992).

54. Measurements of Lorentz-Broadening Coefficients and Pressure-Induced Line Shift Coefficients in the ν_1 band HD¹⁶O and the ν_3 band of D₂¹⁶O.
C. P. Rinsland, M. A. H. Smith, V. Malathy Devi, and D. Chris Benner
J. Mol. Spectrosc. 156, 507 (1993).

55. Measurements of Air-Broadening and Pressure-Shifting of Methane Lines in the 2.3 μm Region.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsland
J. Mol. Spectrosc. 157, 95 (1993).

56. The Hybrid-Type Bands ν_1 and ν_3 of ¹⁶O¹⁶O¹⁷O: Line Positions and Intensities.
M. Heyart, A. Perrin, J. -M. Flaud, C. Camy-Peyret, C. P. Rinsland, M. A. H. Smith, and V. Malathy Devi
J. Mol. Spectrosc. 157, 524 (1993).

57. Air-, N₂- and O₂-Broadening and Shift Coefficients in the ν_3 spectral region of ¹²CH₄.
D. Chris Benner, V. Malathy Devi, M. A. H. Smith, and C. P. Rinsland
J. Quant. Spectrosc. Radiat. Transfer 50, 65 (1993).

58. The Fundamental Bands of H³⁵Cl and H³⁷Cl: Line positions from High-Resolution Laboratory Data.
C. P. Rinsland, M. A. H. Rinsland, A. Goldman, V. Malathy Devi, and D. Chris Benner
J. Mol. Spectrosc. 159, 274 (1993).

59. Line parameters for ozone hot bands in the 3.3- 3- μm region.
J. -M. Flaud, C. Camy-Peyret, A. Perrin, V. Malathy Devi, A. Barbe, S. Bouzza, J. J. Plateaux, C. P. Rinsland, M. A. H. Smith, and A. Goldman
J. Mol. Spectrosc. 160, 378 (1993).

60. Measurements of pressure broadening and shifts of O₃ lines in the 3- μm region.
M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, and E. S. Prochaska
J. Mol. Spectrosc. 164, 239 (1994); Erratum. J. Mol. Spectrosc. 165, 596 (1994).

61. Temperature Dependence of Lorentz air-broadening and pressure-shift coefficients of $^{12}\text{CH}_4$ lines in the 2.3- μm spectral region.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsland
J. Quant. Spectrosc. Radiat. Transfer 51, 439 (1994).
62. A multispectrum nonlinear least squares fitting technique.
D. Chris Benner, C. P. Rinsland, V. Malathy Devi, M. A. H. Smith, and D. Atkins
J. Quant. Spectrosc. Radiat. Transfer 53, 705 (1995).
63. Stretch-Bend Levels of Acetylene: Analysis of the Hot Bands in the 3300 cm^{-1} Region.
Y. A. Sarma, R. D'Cunha, G. Guelachvili, R. Farrenq, V. Malathy Devi, D. Chris Benner, and K. Narahari Rao
J. Mol. Spectrosc. 173, 574 (1995).
64. Infrared Spectroscopy of the CO_2 molecule.
V. Malathy Devi, D. C. Benner, C. P. Rinsland, M. A. H. Smith, and D. S. Parmar
In *Recent Developments in Geophysical Research*, ed. S. G. Pandali, pp. 119-148, Research Signpost, Trivandrum, India (1996).
65. Temperature dependence of air-broadening and shift coefficients of O_3 lines in the ν_1 band.
M. A. H. Smith, V. Malathy Devi, D. Chris Benner, and C. P. Rinsland
J. Mol. Spectrosc. 182, 239-259 (1997).
66. Air-broadening and shift coefficients of O_3 lines in the ν_2 band and their temperature dependence.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
J. Mol. Spectrosc. 182, 221-238 (1997).
67. Air- and N_2 -broadening coefficients and pressure-shift coefficients in the $^{12}\text{C}^{16}\text{O}_2$ laser bands.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
J. Quant. Spectrosc. Radiat. Transfer 59, 137-149 (1998).
68. Absolute rovibrational intensities of $^{12}\text{C}^{16}\text{O}_2$ absorption bands in the 3090 to 3900 cm^{-1} spectral region.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd

J. Quant. Spectrosc. Radiat. Transfer 60, 741-770 (1998).

69. Pressure broadening and pressure shift coefficients in the $2\nu_2^0$ and ν_1 bands of $^{16}\text{O}^{13}\text{C}^{18}\text{O}$.
 V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
 J. Quant. Spectrosc. Radiat. Transfer 60, 771-784 (1998).

70. Spectroscopic Parameters of ozone and its isotopes: Current status, prospects for improvement, and the identification of $^{16}\text{O}^{16}\text{O}^{17}\text{O}$ and $^{16}\text{O}^{17}\text{O}^{16}\text{O}$ lines in infrared ground-based and stratospheric solar absorption spectra.
 C. P. Rinsland, J. -M. Flaud, A. Goldman, A. Perrin, C. Camy Peyret, M. A. H. Smith, V. Malathy Devi, D. C. Benner, A. Barbe, T. M. Stephen, and F. J. Murcray.
 J. Quant. Spectrosc. Radiat. Transfer 60, 803-814 (1998).

71. Self-broadening and self-shift coefficients in the fundamental band of $^{12}\text{C}^{16}\text{O}$.
 V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
 J. Quant. Spectrosc. Radiat. Transfer 60, 815-824 (1998).

72. Measurements of air-broadening, pressure shifting and off-diagonal relaxation-matrix coefficients in the ν_3 band of $^{12}\text{CH}_3\text{D}$.
 V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsalnd, and L. R. Brown
 J. Mol. Structure, in press (2000).

73. Measurements of air broadened width and air-induced shift coefficients and line mixing in the ν_6 band of $^{12}\text{CH}_3\text{D}$.
 V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
 J. Quant. Spectrosc. Radiat. Transfer, in press (2000).

74. Measurements of air broadened width and air-induced shift coefficients and line mixing in the ν_5 band of $^{12}\text{CH}_3\text{D}$.
 V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
 J. Quant. Spectrosc. Radiat. Transfer, in press (2000).

75. Absolute intensities of O_3 lines in the 9-11 μm region.
 M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, and D. C. Benner
 J. Geophys. Res. to be submitted (2000).

List of Contributed Papers: (1995 and onwards) Papers presented prior to 1995 are not included in this list.

1. CO₂ bands in the 3350 - 3700 cm⁻¹ spectral region: Ro-vibrational constants and absolute intensities.

V. Malathy Devi, D. Chris Benner, C. P. Rinsland, and M. A. H. Smith
 Fiftieth International Symposium on Molecular Spectroscopy, p. 105 (1995).

2. Measurements of O₃ line intensities in the ν_3 band: Preliminary results.

M. A. H. Smith, V. Malathy Devi, D. Chris Benner, and C. P. Rinsland
 Fiftieth International Symposium on Molecular Spectroscopy, p. 275 (1995).

3. Vibrational energies and rotational constants of ¹²C¹⁶O₂.

D. Chris Benner, V. Malathy Devi, C. P. Rinsland, and M. A. H. Smith
 Fifty-first International Symposium on Molecular Spectroscopy, p. 102 (1996).

4. Absolute intensities of CO₂ lines in the 1830 to 4000 cm⁻¹ spectral region.

V. Malathy Devi, D. Chris Benner, C. P. Rinsland, and M. A. H. Smith
 Fifty-first International Symposium on Molecular Spectroscopy, p. 102 (1996).

5. Comparison of CO₂ absolute intensities for bands near 4000 cm⁻¹.

D. Chris Benner, Lawrence P. Giver, C. Chackerian, Jr., V. Malathy Devi, L. R. Brown, C. P. Rinsland, and M. A. H. Smith
 Fifty-first International Symposium on Molecular Spectroscopy, p. 103 (1996).

6. Measurements of O₃ line intensities in the ν_3 band.

M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, and D. Chris Benner
 Fifty-first International Symposium on Molecular Spectroscopy, p. 104 (1996).

7. Line intensity measurements in the ν_3 band of O₃.

M. A. H. Smith, V. Malathy Devi, D. Chris Benner, and C. P. Rinsland
 Atmospheric Spectroscopy Applications Workshop, Reims, France Sept. 4-6, 1996

8. Temperature dependence of ozone air-broadening and shift coefficients.
M. A. H. Smith, V. Malathy Devi, D. Chris Benner, and C. P. Rinsland
14th International Conference on High Resolution Molecular Spectroscopy, Prague,
p. 72, Sept. 9-13 (1996).
9. Spectroscopic parameters of CO₂ in the 2.5 to 5.5- μ m spectral region.
V. Malathy Devi, D. Chris Benner, C. P. Rinsland, and M. A. H. Smith
14th International Conference on High Resolution Molecular Spectroscopy, Prague,
p. 113, Sept. 9-13 (1996).
10. Absolute intensities of O₃ lines in the 9-11 μ m region
M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, and D. C. Benner
Fifty-second International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 16-20, 1997. Paper RF03
11. Self-broadening and self-shift coefficients in the 1-0 band of ¹²C¹⁶O
D. Chris Benner, V. Malathy Devi, M. A. H. Smith, and C. P. Rinsland
Fifty-second International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 16-20, 1997. Paper RF05
12. Pressure broadening and pressure shift coefficients in the 2v₂⁰ and v₁ bands of ¹⁶O¹³C¹⁸O.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
Fifty-second International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 16-20, 1997. paper RF13
13. Air- and N₂-broadening coefficients and pressure shift coefficients in the ¹²C¹⁶O₂ laser bands
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
Fifty-second International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 16-20, 1997. Paper RF14
14. Pressure broadening and pressure shift coefficients in the 2v₂⁰ and v₁ bands of ¹⁶O¹³C¹⁸O.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsalnd
15th Colloquim on High Resolution Molecular Spectroscopy, Strathclyde University,
Glasgow, 7-11 September 1997. Poster M7 (p.203)

15. Air- and N₂-broadening coefficients and pressure-shift coefficients in the ¹²C¹⁶O₂ laser bands.
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsland
15th Colloquim on High Resolution Molecular Spectroscopy, Strathclyde University,
Glasgow, 7-11 September 1997. Poster N8 (p. 242)
16. Absolute intensities of O₃ lines in the 9-11 mm
M. A. Smith, C. P. Rinsland, V. Malathy Devi, and D. Chris. Benner
Fifty-third International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 15-19, 1998. Paper WF04
17. Pressure broadening and shift coefficients for water in the 2.5 μ m region
K. Keppler Albert, D. Chris Benner, V. Malathy Devi, and M. A. H. Smith
Fifty-third International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 15-19, 1998. Paper WF06
18. Self- and Air-broadening and shift coefficients of CH₄ lines in the 3 μ m region
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsland, G. Guelachvili,
and L. R. Brown
Fifty-third International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 15-19, 1998. Paper WF11
19. Temperature dependence of air-broadening and shift coefficients in the v₃ band of ¹²CH₄
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsland, G. Guelachvili,
and L. R. Brown
Fifty-third International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 15-19, 1998. Paper WF12
20. Line mixing coefficients in the v₃ band of ¹²CH₄ and ¹³CH₄
D. Chris Benner, V. Malathy Devi, M. A. H. Smith, C. P. Rinsland, G. Guelachvili,
and L. R. Brown
Fifty-third International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 15-19, 1998. Paper WF13
21. Air-Broadening coefficients and pressure shift coefficients of ¹²CH₃D lines in the 7.7 to
10 μ m spectral region

V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and C. P. Rinsland
Fifty-third International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 15-29, 1998. Paper WF14

22. Precise line parameters of methane in the MOPITT CO and methane channels
Adriana Predoi-Cross, V. malathy Devi, D. Chris Benner, Linda R. Brown, Mary Ann H.
Smith, and J. R. Drummond
OSA meeting on Fourier Transform Spectroscopy, June 1999.

23. Assigning Database Broadening and Shift Parameters: O₃ and CH₃D
M. A. H. Smith, V. malathy Devi, D. Chris Benner, and C. P. Rinsland
Proceedings of the Atmospheric Spectroscopy Applications, Universite de Reims,
1-3 September 1999, Poster EP4, p. 229.

24. Temperature dependence of line mixing in the ν_3 band of ¹²CH₄
D. Chris Benner, V. Malathy Devi, M. A. H. Smith, C. P. Rinsland, G. Guelachvili,
and L. R. Brown
Fifty-fourth International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 14-18, 1999. Paper WH02

25. Measurements of air-broadening and pressure-shift coefficients and line mixing in the
 ν_6 fundamental band of ¹²CH₃D
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsland, and L. R. Brown
Fifty-fourth International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 14-18, 1999. Paper WH03

26. Air-broadening and shift coefficients and line mixing in the ν_3 fundamental band of ¹²CH₃D
V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsland, and L. R. Brown
Fifty-fourth International Symposium on Molecular Spectroscopy, Ohio State
University, Columbus, Ohio, June 14-18, 1999. Paper WH04

27. Air-broadening and shift coefficients and line mixing in the ν_3 , ν_5 , and ν_6 bands of ¹²CH₃D
M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, and D. Chris Benner
16th Colloquim on High Resolution Molecular Spectroscopy, Universite de Bourgogne,
Dijon, France, 6-10 September 1999. Poster B23

28. Temperature dependence of pressure-broadening, pressure-shifting and line mixing due to air in the ν_3 band region of $^{12}\text{CH}_4$.
 V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsland, G. Guelachvili, Nathalie Picqué, and L. R. Brown. 16th Colloquim on High Resolution Molecular Spectroscopy, Universite de Bourgogne, Dijon, France, 6-10 September 1999. Poster D23

29. Water Vapor Line Parameters in the 3500-650 cm⁻¹ Region
 K. Keppler Albert, D. Chris Benner, V. Malathy Devi, M. A. H. Smith, and Michael Lock
 16th Colloquim on High Resolution Molecular Spectroscopy, Universite de Bourgogne, Dijon, France, 6-10 September 1999. Poster D26

30. Line Parameters of Methane in the MOPITT Spectral Region
 Adriana Predoi-Cross, J. R. Drummond, V. Malathy Devi, D. Chris Benner, M. A. H. Smith, and L. R. Brown
 16th Colloquim on High Resolution Molecular Spectroscopy, Universite de Bourgogne, Dijon, France, 6-10 September 1999. Post-Deadline Poster, p.4

The following oral presentations are submitted for the 55th Ohio State University International Symposium on Molecular Spectroscopy, to be held in June 2000.

1. High Resolution Spectra of Isotopic Ozone in the 5 μm Region
 M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, D. Chris Benner, T. M. Stephen, A. Goldman and A. Perrin
2. Nitrogen Broadening and Shift Coefficients in the ν_5 and ν_6 fundamental bands of $^{12}\text{CH}_3\text{D}$
 V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsland, L. R. Brown, and R. L. Sams
3. Analysis of self-broadened spectra in the ν_5 and ν_6 fundamental bands of $^{12}\text{CH}_3\text{D}$
 L. R. Brown, V. Malathy Devi, D. Chris Benner, M. A. H. Smith, C. P. Rinsland and R. L. Sams
4. Nitrogen- and Self-Broadening and shift Coefficients in the ν_3 fundamental band of $^{12}\text{CH}_3\text{D}$
 M. A. H. Smith, C. P. Rinsland, V. Malathy Devi, D. Chris Benner and L. R. Brown
5. Line Mixing in the triad of $^{12}\text{CH}_3\text{D}$
 D. Chris Benner, V. Malathy Devi, L. R. Brown, M. A. H. Smith and C. P. Rinsland
6. Temperature Dependence of Line Mixing in the P Branch of the ν_3 Band of Methane
 D. Chris Benner, V. Malathy Devi, M. A. H. Smith, C. P. Rinsland, G. Guelachvili, N. Picqué, and L. R. Brown

7. Measurements of 1-0 Band of Carbon Monoxide at Temperatures between 11 and 296 Kelvins
B. Aoaeh, N. Kolodziejski, A. W. Mantz, D. Chris Benner, V. Malathy Devi, A. H. Smith, C. D. Ball and F. C. DeLucia